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Substrate induced phase transformation of monolayer transition metal dichalcogenides SHUDUN LIU, University of Louisville, XIAOJUN FU, ZHENYU ZHANG, WENGUANG ZHU, University of Science and Technology of China — Using density functional theory calculations, we investigate the effects of a metal substrate on the structural and electronic properties of a monolayer of transition metal dichalcogenide (TMD). We find that a suitable choice of substrate can induce a transformation of the phase of the monolayer from 2H to 1T. We will discuss the impact of the results on some earlier studies of TMD/metal contacts as well as potential applications of our system in catalysis.

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